Journal of Structural Chemistry 2018 vol.59 N2, pages 439-448

Crystal and Molecular Structural Features of Indolin--One Derivatives with Sterically Hindered Phenol Moieties

Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

© 2018, Pleiades Publishing, Ltd. The crystal and molecular structure of four indolin-2-ones with a bulky phenol substituent is studied by single crystal X-ray diffraction. All structures contain a sterically loaded 4-hydroxy-3,5-di-tert-butylbenzyl substituent at the N(1) position of the indole heterocycle. The crystal unit cells of two compounds with the thiosemicarbazone substituent at the C(3) atom of the cycle include one DMSO solvent molecule and the cells of two other molecules with the oxygen atom at the same position do not include solvent molecules. In two of the studied structures the thiosemicarbazone moiety has the Z,E,E configuration favorable for manifestation of the biological activity of these compounds. In three of four molecules the OH group of the bulky substituent at the N(1) atom of the cycle is not involved in hydrogen bonds due to steric hindrances.

http://dx.doi.org/10.1134/S0022476618020270

Keywords

crystal and molecular structure, indolin-2-ones, intermolecular interactions, isatin, single crystal X-ray diffraction, sterically loaded phenols

References

[1] E. T. Denisov and I. B. Afanas'ev. Oxidation and Antioxidants in Organic Chemistry and Biology. Boca Raton: Taylor Francis, 2005.

[2] F. Gugumus. Antioxidants, Plastic additives. 4th ed. Munich: Carl Hanser Verlag, 2001.

[3] V. P. Osipova, M. N. Kolyada, N. T. Berberova, E. R. Milaeva, E. N. Ponomareva, and M. M. Belaya. Cryobiology, 2014, 69,467.

[4] K. D. Breese, J.-F. Lamethe, and C. De Armitt. Polym. Degrad. Stab., 2000, 70,89.

[5] F. Gugumus. Plastics Additives. New York: Oxford University Press, 1990.

[6] G. Kasza, K. Mosnácková, A. Nádor, Z. Osváth, T. Stumphauser, G. Szarka, K. Czaniková, J. Rychlý, Š. Chmela, B. Iván, and J. Mosnácek. Eur. Polym. J., 2015, 68,609.

[7] G. N. Nugumanova, S. V. Bukharov, R. G. Tagasheva, N. A. Mukmeneva, and R. Ya. Deberdeev, Russ. J. Gen. Chem., 2015, 85(1),58.

[8] F. B. Kaynak, S. Ozbey, and N. Karali. J. Mol. Struct., 2013, 1049,157.

[9] A. F. A. M. Mohd, I. M. M. Tahir, K. A. Crouse, F. N.-F. How, and D. J. Watkin. J. Chem. Crystallogr., 2012, 42,173.

[10] G. Kumari and R. K. Singh. Med. Chem. Res., 2013, 22,927.

[11] N. Karali, A. Gürsoy, F. Kandemirli, N. Shvets, F. Betül Kaynak, S. Özbey, V. Kovalishyn, and A. Dimoglo. Bioorg. Med. Chem., 2007, 15, 5888.

[12] P. Diaz, Sh. S. Phatak, F. Astruc-Diaz, J. Xu, C. N. Cavasotto, and M. Naguib. J. Med. Chem., 2009, 52,433.

[13] P. Diaz, J. Xu, F. Astruc-Diaz, H.-M. Pan, D. L. Brown, and M. Naguib. J. Med. Chem., 2008, 51, 4932.

[14] M. C. Rodríguez-Argüelles, S. Mosquera-Vázquez, P. Tourón-Touceda, J. Sanmartín-Matalobos, A. M. García-Deibe, M. Belicchi-Ferrari, G. Pelosi, C. Pelizzi, and F. Zani. J. Inorg. Biochem., 2007, 101,138.

[15] M. C. Rodríguez-Argüelles, R. Cao, A. M. García-Deibe, C. Pelizzi, J. Sanmartín-Matalobos, and F. Zani. Polyhedron, 2009, 28, 2187.

[16] K. Mamari, A. Zerzouf, H. Zouihri, E. M. Essassia, and S. W. Ng. Acta Crystallogr. E., 2010, 66, o1332.

[17] A. Alsubari, A. Moussaif, H. Zouihri, E. M. Essassia, and S. W. Ng. Acta Crystallogr. E., 2010, 66, o1905.

[18] G. Pelosi, C. Pelizzi, M. Belicchi Ferrari, M. C. Rodriguez-Arguelles, C. Vieitob, and J. Sanmartin. Acta Crystallogr. C, 2005, 61, o589.

[19] R. Mudududdla, R. Sharma, S. K. Guru, M. Kushwaha, A. P. Gupta, S. S. Bharate, S. Aravinda, R. Kant, Sh. Bhushan, R. A. Vishwakarma, and S. B. Bharate. RSC Adv., 2014, 4, 14081.

[20] A. V. Bogdanov, S. V. Bukharov, Yu. N. Oludina, L. I. Musin, G. N. Nugumanova, V. V. Syakaev, and V. F. Mironov. ARKIVOC, 2013, iii,424.

[21] Cambrige Structural Database System, Version 5.34, Cambridge Crystallographic Data Centre, 2013.

[22] APEX2, Version 2.1, SAINTPlus, Data Reduction and Correction Program, Version 7.31A, Bruker Advansed X-ray Solutions, BrukerAXS Inc., Madison, Wisconsin, USA, 2006.

[23] G. M. Sheldrik. SADABS, Program for empirical X-ray absorption correction, Bruker-Nonius, 1990-2004.

[24] G. M. Sheldrik. Acta Crystallogr. A, 2008, 64,112.

[25] L. J. Farrugia. J. Appl. Crystallogr., 1999, 32,837.

[26] A. L. Spek. Acta Crystallogr. D, 2009, 65,148.

[27] F. H. Allen, O. Kennard, D. G. Watson, L. Brammer, A. G. Orpen, and R. Taylor. J. Chem. Soc. Perkin Trans., 1987,1.

[28] E. V. Mironova, A. V. Bogdanov, D. B. Krivolapov, L. I. Musin, I. A. Litvinov, and V. F. Mironov. J. Mol. Struct., 2015, 1079,87.

[29] Ho Soo Yei, R. P. A. Bettens, D. Dakternieks, A. Duthieb, and E. R. T. Tiekink. CrystEngComm, 2005, 7,682.

[30] A. Saeeda, M. F. Erbenb, U. Shaheena, and U. Flurke. J. Mol. Struct., 2011, 1000,49.

[31] E. M. Fleming, T. McCabe, and S. J. Connon. Tetrahedron Lett., 2006, 47, 7037.

[32] E. S. Raper, J. R. Creighton, and R. E. Oughtredet. Acta Crystallogr., 1983, B39,355.

[33] G. Vampa, S. Benvenuti, and F. Severiet. J. Heterocycl. Chem., 1995, 32,227.

[34] O. A. Lodochnikova, A. V. Bodrov, A. F. Saifina, L. E. Nikitina, and I. A. Litvinov, J. Struct. Chem., 2013, 54(1), 140–147.